

Spectral Properties of p -Sombor Matrices and Beyond

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Abstract

Let $G = (V(G), E(G))$ be a simple graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G)$. The p -Sombor matrix $\mathcal{S}_p(G)$ of G is the square matrix of order n whose (i, j) -entry is equal to $((d_i)^p + (d_j)^p)^{\frac{1}{p}}$ if $v_i \sim v_j$, and 0 otherwise, where d_i denotes the degree of vertex v_i in G . In this paper, we study the relationship between p -Sombor index $SO_p(G)$ and p -Sombor matrix $\mathcal{S}_p(G)$ by the k -th spectral moment N_k and the spectral radius of $\mathcal{S}_p(G)$. Then we obtain some bounds of p -Sombor Laplacian eigenvalues, p -Sombor spectral radius, p -Sombor spectral spread, p -Sombor energy and p -Sombor Estrada index. We also investigate the Nordhaus-Gaddum-type results for p -Sombor spectral radius and energy. At last, we give the regression model for boiling point and some other invariants.

1 Introduction

Let $G = (V(G), E(G))$ be a simple graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G)$. Let d_i be the degree of vertex $v_i \in V(G)$, $i \sim j$ denote $v_i v_j \in E(G)$. In this paper, for all notations and terminologies used, but not defined here, we refer to the textbook [3].

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Based on elementary geometry, a novel vertex-degree-based topological index, the Sombor index was introduced by Gutman in chemical graph theory, which is defined as [24]

$$SO(G) = \sum_{v_i v_j \in E(G)} \sqrt{d_i^2 + d_j^2} \triangleq \sum_{\substack{i \sim j \\ 1 \leq i, j \leq n}} \sqrt{d_i^2 + d_j^2}.$$

See [1, 5–8, 10–13, 15, 18, 21, 22, 24, 25, 28, 30–34, 36, 38, 40, 44] for more details.

This form of the Sombor index corresponds to a 2-norm, and it is a natural idea to define a more general form, i.e., p -norm. With this in mind, Réti, Došlić and Ali [38], proposed the p -Sombor index ($p \neq 0$), which was defined as

$$SO_p(G) = \sum_{v_i v_j \in E(G)} ((d_i)^p + (d_j)^p)^{\frac{1}{p}} \triangleq \sum_{\substack{i \sim j \\ 1 \leq i, j \leq n}} ((d_i)^p + (d_j)^p)^{\frac{1}{p}}.$$

It obvious that SO_1 is the first Zagreb index [19], SO_2 is the Sombor index, SO_{-1} is the inverse sum indeg index (ISI index) [42].

As we know, the adjacent matrix $A(G) = [a_{ij}]_{n \times n}$ is defined as

$$a_{ij} = \begin{cases} 1, & v_i v_j \in E(G); \\ 0, & otherwise. \end{cases}$$

The adjacent eigenvalues with non-increasing order are $\mu_1 \geq \mu_2 \geq \dots \geq \mu_n$.

The concept of graph energy was firstly introduced by Gutman [23], which is defined as

$$\mathcal{E}(G) = \sum_{i=1}^n |\mu_i|.$$

Due to the importance of the concept of energy, it is widely studied in computational chemistry. We can refer to [2, 9] for more details about energy.

Let G be a simple graph. We define the p -Sombor matrix as $\mathcal{S}_p = \mathcal{S}_p(G) = [s_{ij}^p]_{n \times n}$ ($p \neq 0$), where

$$s_{ij}^p = \begin{cases} ((d_i)^p + (d_j)^p)^{\frac{1}{p}}, & v_i v_j \in E(G); \\ 0, & otherwise. \end{cases}$$

It is obvious that $SO_p(G) = \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n s_{ij}^p$.

Let $\xi_1 \geq \xi_2 \geq \dots \geq \xi_n$ be the eigenvalues of \mathcal{S}_p . We call $\xi_1 \geq \xi_2 \geq \dots \geq \xi_n$ the p -Sombor eigenvalues of G , ξ_1 the p -Sombor spectral radius of G and $\xi_1 - \xi_n$ the spectral spread of \mathcal{S}_p .

The p -Sombor energy $S_p E$ and the p -Sombor Estrada index $S_p EE$ of G are defined as

$$S_p E = S_p E(G) = \sum_{i=1}^n |\xi_i|, \quad S_p EE = S_p EE(G) = \sum_{i=1}^n e^{\xi_i},$$

respectively, and the p -Sombor Laplacian matrix of G is defined as

$$\mathcal{L}_p(G) = \mathcal{D}_p(G) - \mathcal{S}_p(G),$$

where $\mathcal{D}_p(G) = \text{Diag}(\sum_{k=1}^n s_{1k}^p, \sum_{k=1}^n s_{2k}^p, \dots, \sum_{k=1}^n s_{nk}^p)$.

It is worth noting that the p -Sombor matrix (weighted adjacency matrices) behaves quite different from the traditional adjacency matrix, for example, the p -Sombor spectral radius has no monotonicity [29]. This is the reason why we propose this class of matrices.

The rest of the paper is organized as follows. In Section 2, we study the relationship between p -Sombor index $SO_p(G)$ and p -Sombor matrix $\mathcal{S}_p(G)$ by the k -th spectral moment N_k and the spectral radius of $\mathcal{S}_p(G)$. In Section 3, we obtain some bounds of p -Sombor Laplacian eigenvalues. In Section 4, we consider some bounds of p -Sombor spectral radius and p -Sombor spectral spread. In Section 5, we investigate some bounds of p -Sombor energy and p -Sombor Estrada index. In Section 6, we study the Nordhaus-Gaddum-type results for p -Sombor spectral radius and energy. In Section 7, we give the regression model for boiling point and some other invariants. In Section 8, we conclude this paper and propose some open problems.

2 Relationship between the p -Sombor matrix $\mathcal{S}_p(G)$ and the p -Sombor index $SO_p(G)$

Let G be a simple graph, $\mathcal{S}_p = \mathcal{S}_p(G)$, N_k be the k -th spectral moment of \mathcal{S}_p , i.e., $N_k = \sum_{i=1}^n (\xi_i)^k$. It is obvious that $N_k = \text{tr}((\mathcal{S}_p)^k)$, thus $S_p EE(G) = \sum_{k=0}^{\infty} \frac{N_k}{k!}$.

Lemma 2.1 *Let G be a graph with $|V(G)| = n$ and $\mathcal{S}_p = \mathcal{S}_p(G)$ be the p -Sombor matrix of G . Then*

- (1) $N_0 = n$;
- (2) $N_1 = 0$;
- (3) $N_2 = 2 \sum_{\substack{i \sim j \\ 1 \leq i, j \leq n}} ((d_i)^p + (d_j)^p)^{\frac{2}{p}}$;
- (4) $N_3 = 2 \sum_{\substack{i \sim j \\ 1 \leq i, j \leq n}} \left(((d_i)^p + (d_j)^p)^{\frac{1}{p}} \sum_{\substack{j \sim k, k \sim i \\ 1 \leq k \leq n}} ((d_i)^p + (d_k)^p)^{\frac{1}{p}} ((d_k)^p + (d_j)^p)^{\frac{1}{p}} \right)$;

$$(5) N_4 = \sum_{i=1}^n \left(\sum_{\substack{i \sim j \\ 1 \leq j \leq n}} ((d_i)^p + (d_j)^p)^{\frac{2}{p}} \right)^2 + \sum_{i \neq j} \left(\sum_{\substack{k \sim i, k \sim j \\ 1 \leq k \leq n}} ((d_i)^p + (d_k)^p)^{\frac{1}{p}} ((d_j)^p + (d_k)^p)^{\frac{1}{p}} \right)^2;$$

Proof. (1) $N_0 = \sum_{i=1}^n (\xi_i)^0 = n$.

$$(2) N_1 = \text{tr}(\mathcal{S}_p) = 0.$$

(3) For any $1 \leq i, j \leq n$ and $i \neq j$, we have

$$\begin{aligned} ((\mathcal{S}_p)^2)_{ij} &= \sum_{k=1}^n (\mathcal{S}_p)_{ik} (\mathcal{S}_p)_{kj} = \sum_{\substack{k \sim i, k \sim j \\ 1 \leq k \leq n}} (\mathcal{S}_p)_{ik} (\mathcal{S}_p)_{kj} \\ &= \sum_{\substack{k \sim i, k \sim j \\ 1 \leq k \leq n}} ((d_i)^p + (d_k)^p)^{\frac{1}{p}} ((d_k)^p + (d_j)^p)^{\frac{1}{p}}. \end{aligned}$$

For any $1 \leq i \leq n$, we have

$$((\mathcal{S}_p^2)_{ii}) = \sum_{j=1}^n (\mathcal{S}_p)_{ij} (\mathcal{S}_p)_{ji} = \sum_{\substack{i \sim j \\ 1 \leq j \leq n}} ((\mathcal{S}_p)_{ij})^2 = \sum_{\substack{i \sim j \\ 1 \leq j \leq n}} ((d_i)^p + (d_j)^p)^{\frac{2}{p}}.$$

Thus

$$N_2 = \text{tr}((\mathcal{S}_p)^2) = \sum_{i=1}^n \left(\sum_{\substack{i \sim j \\ 1 \leq j \leq n}} ((d_i)^p + (d_j)^p)^{\frac{2}{p}} \right) = 2 \sum_{\substack{i \sim j \\ 1 \leq i, j \leq n}} ((d_i)^p + (d_j)^p)^{\frac{2}{p}}.$$

(4) For any $1 \leq i \leq n$, we have

$$\begin{aligned} ((\mathcal{S}_p^3)_{ii}) &= \sum_{j=1}^n (\mathcal{S}_p)_{ij} ((\mathcal{S}_p^2)_{ji}) = \sum_{\substack{i \sim j \\ 1 \leq j \leq n}} ((d_i)^p + (d_j)^p)^{\frac{1}{p}} ((\mathcal{S}_p^2)_{ji}) \\ &= \sum_{\substack{i \sim j \\ 1 \leq j \leq n}} \left(((d_i)^p + (d_j)^p)^{\frac{1}{p}} \times \sum_{\substack{j \sim k, k \sim i \\ 1 \leq k \leq n}} ((d_i)^p + (d_k)^p)^{\frac{1}{p}} ((d_k)^p + (d_j)^p)^{\frac{1}{p}} \right). \end{aligned}$$

Thus

$$\begin{aligned} N_3 &= \text{tr}((\mathcal{S}_p^3)) = \sum_{i=1}^n (((\mathcal{S}_p^3)_{ii})) \\ &= \sum_{i=1}^n \left(\sum_{\substack{i \sim j \\ 1 \leq j \leq n}} \left(((d_i)^p + (d_j)^p)^{\frac{1}{p}} \sum_{\substack{j \sim k, k \sim i \\ 1 \leq k \leq n}} ((d_i)^p + (d_k)^p)^{\frac{1}{p}} ((d_k)^p + (d_j)^p)^{\frac{1}{p}} \right) \right) \\ &= 2 \sum_{\substack{i \sim j \\ 1 \leq i, j \leq n}} \left(((d_i)^p + (d_j)^p)^{\frac{1}{p}} \sum_{\substack{j \sim k, k \sim i \\ 1 \leq k \leq n}} ((d_i)^p + (d_k)^p)^{\frac{1}{p}} ((d_k)^p + (d_j)^p)^{\frac{1}{p}} \right). \end{aligned}$$

(5) Since $\text{tr}((\mathcal{S}_p)^4) = \|(\mathcal{S}_p)^2\|_F^2$, where $\|(\mathcal{S}_p)^2\|_F$ is the Frobenius norm of $(\mathcal{S}_p)^2$, thus

$$\begin{aligned} N_4 = \text{tr}((\mathcal{S}_p)^4) &= \sum_{i,j=1}^n \left(((\mathcal{S}_p^2)_{ij})^2 \right) = \sum_{i=j} \left(((\mathcal{S}_p^2)_{ij})^2 \right) + \sum_{i \neq j} \left(((\mathcal{S}_p^2)_{ij})^2 \right) \\ &= \sum_{i=1}^n \left(\sum_{\substack{i \sim j \\ 1 \leq j \leq n}} \left((d_i)^p + (d_j)^p \right)^{\frac{2}{p}} \right)^2 + \sum_{i \neq j} \left(\sum_{\substack{k \sim i, k \sim j \\ 1 \leq k \leq n}} \left((d_i)^p + (d_k)^p \right)^{\frac{1}{p}} \left((d_k)^p + (d_j)^p \right)^{\frac{1}{p}} \right)^2. \end{aligned}$$

■

In the following, we obtain some bounds of the p -Sombor spectral moment.

Theorem 2.2 *Let G be a graph with $|E(G)| = m$ and the maximum (resp. minimum) degree Δ (resp. δ), $SO_p(G)$ be the p -Sombor index of G , N_2 be the 2-th p -Sombor spectral moment. Then*

$$\sqrt{\frac{1}{2}N_2 + 2^{\frac{2}{p}}\delta^2 m(m-1)} \leq SO_p(G) \leq \sqrt{\frac{1}{2}N_2 + 2^{\frac{2}{p}}\Delta^2 m(m-1)},$$

with equality if and only if G is a regular graph.

Proof. By Lemma 2.1, we have

$$\begin{aligned} (SO_p(G))^2 &= \left(\sum_{v_i v_j \in E(G)} \left((d_i)^p + (d_j)^p \right)^{\frac{1}{p}} \right)^2 \\ &= \sum_{i \sim j} \left((d_i)^p + (d_j)^p \right)^{\frac{2}{p}} + \sum_{\substack{i \sim j, k \sim l \\ v_i v_j \neq v_k v_l}} \left((d_i)^p + (d_j)^p \right)^{\frac{1}{p}} \left((d_k)^p + (d_l)^p \right)^{\frac{1}{p}} \\ &= \frac{1}{2}N_2 + \sum_{\substack{i \sim j, k \sim l \\ v_i v_j \neq v_k v_l}} \left((d_i)^p + (d_j)^p \right)^{\frac{1}{p}} \left((d_k)^p + (d_l)^p \right)^{\frac{1}{p}} \\ &\leq \frac{1}{2}N_2 + 2^{\frac{2}{p}}\Delta^2 m(m-1). \end{aligned}$$

Thus, $SO_p(G) \leq \sqrt{\frac{1}{2}N_2 + 2^{\frac{2}{p}}\Delta^2 m(m-1)}$, with equality if and only if G is a regular graph. Similarly, we have $SO_p(G) \geq \sqrt{\frac{1}{2}N_2 + 2^{\frac{2}{p}}\delta^2 m(m-1)}$, with equality if and only if G is a regular graph. ■

Theorem 2.3 *Let G be a graph with the maximum (resp. minimum) degree Δ (resp. δ), $SO_p(G)$ be the p -Sombor index of G , N_2 be the 2-th p -Sombor spectral moment. Then*

$$\frac{N_2}{2^{(1+\frac{1}{p})}\Delta} \leq SO_p(G) \leq \frac{N_2}{2^{(1+\frac{1}{p})}\delta},$$

with equality if and only if G is a regular graph.

Proof. By Lemma 2.1, we have

$$\begin{aligned} N_2 = \text{tr}(\mathcal{S}_p)^2 &= 2 \sum_{i \sim j} ((d_i)^p + (d_j)^p)^{\frac{2}{p}} \\ &\geq 2^{(1+\frac{1}{p})} \delta \sum_{i \sim j} ((d_i)^p + (d_j)^p)^{\frac{1}{p}} = 2^{(1+\frac{1}{p})} \delta SO_p(G). \end{aligned}$$

Thus, $SO_p(G) \leq \frac{N_2}{2^{(1+\frac{1}{p})} \delta}$, with equality if and only if G is a regular graph.

Similarly, $SO_p(G) \geq \frac{N_2}{2^{(1+\frac{1}{p})} \Delta}$, with equality if and only if G is a regular graph. \blacksquare

Let $N(u)$ be the set of neighbors of vertex u in G , $t_{\max} = \max_{uv \in E(G)} |N(u) \cap N(v)|$ and $t_{\min} = \min_{uv \in E(G)} |N(u) \cap N(v)|$.

Theorem 2.4 *Let G be a graph with $t_{\max}, t_{\min} \geq 1$, $SO_p(G)$ be the p -Sombor index of G , N_3 be the 3-th p -Sombor spectral moment. Then*

$$\frac{N_3}{2^{(1+\frac{2}{p})} \Delta^2 t_{\max}} \leq SO_p(G) \leq \frac{N_3}{2^{(1+\frac{2}{p})} \delta^2 t_{\min}},$$

with equality if and only if G is a regular graph and $t_{\max} = t_{\min}$.

Proof. By Lemma 2.1, we have

$$\begin{aligned} N_3 = \text{tr}((\mathcal{S}_p)^3) &= 2 \sum_{\substack{i \sim j \\ 1 \leq i, j \leq n}} \left(((d_i)^p + (d_j)^p)^{\frac{1}{p}} \sum_{\substack{k \sim i, k \sim j \\ 1 \leq k \leq n}} ((d_i)^p + (d_k)^p)^{\frac{1}{p}} ((d_k)^p + (d_j)^p)^{\frac{1}{p}} \right) \\ &\geq 2^{(1+\frac{2}{p})} \delta^2 \sum_{\substack{i \sim j \\ 1 \leq i, j \leq n}} \left(((d_i)^p + (d_j)^p)^{\frac{1}{p}} \sum_{\substack{k \sim i, k \sim j \\ 1 \leq k \leq n}} 1 \right) \\ &\geq 2^{(1+\frac{2}{p})} \delta^2 t_{\min} \sum_{\substack{i \sim j \\ 1 \leq i, j \leq n}} ((d_i)^p + (d_j)^p)^{\frac{1}{p}} \\ &= 2^{(1+\frac{2}{p})} \delta^2 t_{\min} SO_p(G). \end{aligned}$$

Thus, $SO_p(G) \leq \frac{N_3}{2^{(1+\frac{2}{p})} \delta^2 t_{\min}}$, with equality if and only if G is a regular graph and any two adjacent vertices have the same number of common neighbours, then G is a regular graph and $t_{\max} = t_{\min}$. Similarly, we also have $SO_p(G) \geq \frac{N_3}{2^{(1+\frac{2}{p})} \Delta^2 t_{\max}}$, with equality if and only if G is a regular graph and $t_{\max} = t_{\min}$. \blacksquare

Theorem 2.5 *Let G be a graph with $|V(G)| = n$, $|E(G)| = m$, the maximum (resp. minimum) degree Δ (resp. δ), $M_1(G)$ be the first Zagreb index of G , N_4 be the 4-th p -Sombor spectral moment. Then*

$$\frac{N_4 - 2^{\frac{4}{p}} \Delta^5 (M_1(G) - 2m)}{2^{(1+\frac{3}{p})} \Delta^4} \leq SO_p(G) \leq \frac{N_4 - 2^{\frac{4}{p}} \delta^4 (M_1(G) - 2m)}{2^{(1+\frac{3}{p})} \delta^4},$$

with left equality iff $G \cong K_{\Delta, \Delta}$, with right equality iff G is a δ -regular graph without C_4 .

Proof. Let $|P_3|$ be the numbers of path with length 2 in G . Then

$$|P_3| = \sum_{1 \leq i \leq n} \binom{d_i}{2} = \frac{1}{2} \sum_{1 \leq i \leq n} d_i^2 - \frac{1}{2} \sum_{1 \leq i \leq n} d_i = \frac{1}{2} M_1(G) - m,$$

thus

$$\sum_{\substack{1 \leq i, j \leq n \\ i \neq j}} \left(\sum_{\substack{k \sim i, k \sim j \\ 1 \leq k \leq n}} 1 \right) = 2|P_3| = M_1(G) - 2m.$$

Recalling that

$$N_4 = \sum_{i=1}^n \left(\sum_{\substack{i \sim j \\ 1 \leq j \leq n}} ((d_i)^p + (d_j)^p)^{\frac{2}{p}} \right)^2 + \sum_{i \neq j} \left(\sum_{\substack{k \sim i, k \sim j \\ 1 \leq k \leq n}} ((d_i)^p + (d_k)^p)^{\frac{1}{p}} ((d_j)^p + (d_k)^p)^{\frac{1}{p}} \right)^2,$$

then we have

$$\begin{aligned} & \sum_{i=1}^n \left(\sum_{\substack{i \sim j \\ 1 \leq j \leq n}} ((d_i)^p + (d_j)^p)^{\frac{2}{p}} \right)^2 \\ & \leq \sum_{i=1}^n \left(2^{\frac{1}{p}} \Delta \sum_{\substack{i \sim j \\ 1 \leq j \leq n}} ((d_i)^p + (d_j)^p)^{\frac{1}{p}} \right)^2 \\ & \leq 2^{\frac{3}{p}} \Delta^3 \sum_{i=1}^n \left(\left(\sum_{\substack{i \sim j \\ 1 \leq j \leq n}} ((d_i)^p + (d_j)^p)^{\frac{1}{p}} \right) \left(\sum_{\substack{i \sim j \\ 1 \leq j \leq n}} 1 \right) \right) \\ & = 2^{\frac{3}{p}} \Delta^3 \sum_{i=1}^n d_i \left(\sum_{\substack{i \sim j \\ 1 \leq j \leq n}} ((d_i)^p + (d_j)^p)^{\frac{1}{p}} \right) \\ & \leq 2^{(1+\frac{3}{p})} \Delta^4 SO_p(G). \end{aligned}$$

Similarly, we have

$$\sum_{i=1}^n \left(\sum_{\substack{i \sim j \\ 1 \leq j \leq n}} ((d_i)^p + (d_j)^p)^{\frac{2}{p}} \right)^2 \geq 2^{(1+\frac{3}{p})} \delta^4 SO_p(G).$$

On the other hand, we have

$$\begin{aligned}
& \sum_{i \neq j} \left(\sum_{\substack{k \sim i, k \sim j \\ 1 \leq k \leq n}} ((d_i)^p + (d_k)^p)^{\frac{1}{p}} ((d_j)^p + (d_k)^p)^{\frac{1}{p}} \right)^2 \\
& \leq 2^{\frac{4}{p}} \Delta^4 \sum_{i \neq j} \left(\sum_{\substack{k \sim i, k \sim j \\ 1 \leq k \leq n}} 1 \right) \left(\sum_{\substack{k \sim i, k \sim j \\ 1 \leq k \leq n}} 1 \right) \\
& = 2^{\frac{4}{p}} \Delta^4 \sum_{i \neq j} \left(\sum_{\substack{k \sim i, k \sim j \\ 1 \leq k \leq n}} 1 \right) |N(u_i) \cap N(u_j)| \\
& \leq 2^{\frac{4}{p}} \Delta^5 \sum_{i \neq j} \left(\sum_{\substack{k \sim i, k \sim j \\ 1 \leq k \leq n}} 1 \right) \\
& = 2^{\frac{4}{p}} \Delta^5 (M_1(G) - 2m).
\end{aligned}$$

We also have

$$\begin{aligned}
& \sum_{i \neq j} \left(\sum_{\substack{k \sim i, k \sim j \\ 1 \leq k \leq n}} ((d_i)^p + (d_k)^p)^{\frac{1}{p}} ((d_j)^p + (d_k)^p)^{\frac{1}{p}} \right)^2 \\
& \geq 2^{\frac{4}{p}} \delta^4 \sum_{i \neq j} \left(\sum_{\substack{k \sim i, k \sim j \\ 1 \leq k \leq n}} 1 \right) \left(\sum_{\substack{k \sim i, k \sim j \\ 1 \leq k \leq n}} 1 \right) \\
& = 2^{\frac{4}{p}} \delta^4 \sum_{i \neq j} \left(\sum_{\substack{k \sim i, k \sim j \\ 1 \leq k \leq n}} 1 \right) |N(u_i) \cap N(u_j)| \\
& \geq 2^{\frac{4}{p}} \delta^4 \sum_{i \neq j} \left(\sum_{\substack{k \sim i, k \sim j \\ 1 \leq k \leq n}} 1 \right) \\
& = 2^{\frac{4}{p}} \delta^4 (M_1(G) - 2m).
\end{aligned}$$

In summary, we have

$$\frac{N_4 - 2^{\frac{4}{p}} \Delta^5 (M_1(G) - 2m)}{2^{(1+\frac{3}{p})} \Delta^4} \leq SO_p(G) \leq \frac{N_4 - 2^{\frac{4}{p}} \delta^4 (M_1(G) - 2m)}{2^{(1+\frac{3}{p})} \delta^4}.$$

In the following, we consider the sufficient and necessary conditions of the equalities hold.

For the lower bound, the equality holds if and only if $d_i = \Delta$ for all $1 \leq i \leq n$ and $|N(u_i) \cap N(u_j)| = \Delta$, thus $G \cong K_{\Delta, \Delta}$.

For the upper bound, the equality holds if and only if $d_i = \delta$ for all $1 \leq i \leq n$ and $|N(u_i) \cap N(u_j)| = 1$ or 0 , thus G is a δ -regular graph without C_4 . ■

In the following, we obtain more bounds about p -Sombor index. From the definition of p -Sombor index, we immediately have

Lemma 2.6 *Let G be a connected graph with $|V(G)| = n$. Then*

$$SO_p(G) \leq 2^{\frac{1}{p}-1} n(n-1)^2,$$

with equality if and only if $G \cong K_n$.

Theorem 2.7 *Let G be a graph with $|V(G)| = n$. Then*

$$\frac{n\xi_1^2}{2^{(1+\frac{1}{p})}\Delta(n-1)} \leq SO_p(G) \leq \frac{n\xi_1}{2},$$

the left equality holds if $G \cong K_n$, the right equality holds if G is a regular graph.

Proof. Let $e = (1, 1, \dots, 1)^T \in R^n$, ξ_1 be the p -Sombor spectral radius of G . Then

$$\xi_1 = \max_{X \neq 0} \frac{X^T \mathcal{S}_p X}{X^T X} \geq \frac{e^T \mathcal{S}_p e}{e^T e} = \frac{2SO_p(G)}{n},$$

thus $SO_p(G) \leq \frac{n\xi_1}{2}$. If G is a k -regular graph, then $S_p(G) = 2^{\frac{1}{p}} kA(G)$, thus $\xi_1 = 2^{\frac{1}{p}} k\mu_1 = 2^{\frac{1}{p}} k^2$, and $SO_p(G) = (\frac{kn}{2})(2^{\frac{1}{p}} k) = \frac{n\xi_1}{2}$.

On the other hand, we have

$$\xi_1^2 = \left(\sum_{i=2}^n \xi_i \right)^2 \leq (n-1) \left(\sum_{i=2}^n \xi_i^2 \right),$$

then by Theorem 2.3, we have

$$\frac{n\xi_1^2}{n-1} = \xi_1^2 + \frac{\xi_1^2}{n-1} \leq \xi_1^2 + \sum_{i=2}^n \xi_i^2 = \sum_{i=1}^n \xi_i^2 = N_2 \leq 2^{(1+\frac{1}{p})}\Delta SO_p(G).$$

Thus, we have $SO_p(G) \geq \frac{n\xi_1^2}{2^{(1+\frac{1}{p})}\Delta(n-1)}$. If $G \cong K_n$, then $S_p(G) = 2^{\frac{1}{p}}(n-1)A(G)$, thus $\xi_1 = 2^{\frac{1}{p}}(n-1)\mu_1 = 2^{\frac{1}{p}}(n-1)^2$, and $SO_p(G) = (\frac{(n-1)n}{2})(2^{\frac{1}{p}}(n-1)) = \frac{n\xi_1^2}{2^{(1+\frac{1}{p})}\Delta(n-1)}$. ■

Theorem 2.8 *Let G be a graph with $|E(G)| = m$, σ^2 be the variance of $((d_i)^p + (d_j)^p)^{\frac{1}{p}}$ appearing in $SO_p(G)$. Then*

$$SO_p(G) = \sqrt{\frac{1}{2}mN_2 - m^2\sigma^2}.$$

Proof. By the definition of variance and $N_2 = 2 \sum_{\substack{i \sim j \\ 1 \leq i, j \leq n}} ((d_i)^p + (d_j)^p)^{\frac{2}{p}}$, we have

$$\begin{aligned} \sigma^2 &= \frac{1}{m} \sum_{\substack{i \sim j \\ 1 \leq i, j \leq n}} ((d_i)^p + (d_j)^p)^{\frac{2}{p}} - \left(\frac{1}{m} \sum_{\substack{i \sim j \\ 1 \leq i, j \leq n}} ((d_i)^p + (d_j)^p)^{\frac{2}{p}} \right)^2 \\ &= \frac{N_2}{2m} - \frac{(SO_p(G))^2}{m^2}. \end{aligned}$$

Thus, we have $SO_p(G) = \sqrt{\frac{1}{2}mN_2 - m^2\sigma^2}$. ■

The ISI index was defined as $ISI(G) = \sum_{v_i v_j \in E(G)} \frac{d_i d_j}{d_i + d_j}$. We can obtain the relationship between the p -Sombor index $SO_p(G)$ and ISI index $ISI(G)$.

Theorem 2.9 *Let G be a simple graph. Then*

$$SO_p(G) \geq 2^{\left(\frac{1}{p}+1\right)} ISI(G),$$

with equality if and only if G is a regular graph.

Proof. Recalling the Cauchy-Schwarz inequality,

$$\left| \sum_{i=1}^n a_i b_i \right| \leq \left(\sum_{i=1}^n (a_i)^p \right)^{\frac{1}{p}} \left(\sum_{i=1}^n (b_i)^q \right)^{\frac{1}{q}},$$

where $\frac{1}{p} + \frac{1}{q} = 1$ and with equality if and only if $a_i = \lambda b_i$ for any i , λ is a constant.

Then $d_i + d_j \leq 2^{(1-\frac{1}{p})} ((d_i)^p + (d_j)^p)^{\frac{1}{p}}$, thus $((d_i)^p + (d_j)^p)^{\frac{1}{p}} \geq 2^{\frac{1}{p}-1} (d_i + d_j) = 2^{\left(\frac{1}{p}+1\right)} \frac{d_i d_j}{d_i + d_j}$. $\frac{(d_i + d_j)^2}{4d_i d_j} \geq 2^{\left(\frac{1}{p}+1\right)} \frac{d_i d_j}{d_i + d_j}$. So $SO_p(G) \geq 2^{\left(\frac{1}{p}+1\right)} ISI(G)$, with equality if and only if $d_i = d_j$ for every $v_i v_j \in E(G)$, i.e., G is a regular graph. ■

3 Bounds of p -Sombor Laplacian eigenvalues

Suppose the distinct eigenvalues of $\mathcal{L}_p(G)$ are $\eta_1 > \eta_2 > \dots > \eta_s$ and their multiplicities are $m(\eta_1), m(\eta_2), \dots, m(\eta_s)$, respectively. In other words, the spectrum of $\mathcal{L}_p(G)$ is

$$\left(\begin{array}{cccc} \eta_1 & \eta_2 & \dots & \eta_s \\ m(\eta_1) & m(\eta_2) & \dots & m(\eta_s) \end{array} \right).$$

In this section, we consider the relationship between p -Sombor Laplacian eigenvalues and p -Sombor index of G .

Similar to the properties of Laplacian matrix, we also have

Lemma 3.1 *For the matrix $\mathcal{L}_p(G)$, we have $\eta_s = 0$ and $m(\eta_s) = 1$.*

Since p -Sombor Laplacian matrix $\mathcal{L}_p(G)$ is also a non-negative symmetric and irreducible matrix, similarly with the results of [17,37], we also have

Lemma 3.2 *Let G be a simple graph with $|V(G)| = n$, $\mathcal{L}_p(G)$ be the p -Sombor Laplacian matrix of graph G , the distinct eigenvalues of $\mathcal{L}_p(G)$ be $\eta_1 > \eta_2 > \dots > \eta_s$, $e = (1, 1, \dots, 1)^T \in R^n$. Then*

$$(1) \eta_1 = 2n \max \left\{ \frac{\sum_{v_i v_j \in E(G)} s_{ij}^p (\omega_i - \omega_j)^2}{\sum_{v_i \in V(G)} \sum_{v_j \in V(G)} (\omega_i - \omega_j)^2} \mid \omega = (\omega_1, \omega_2, \dots, \omega_n) \in R^n, \omega \neq ae, \forall a \in R \right\};$$

$$(2) \eta_{s-1} = 2n \min \left\{ \frac{\sum_{v_i v_j \in E(G)} s_{ij}^p (\omega_i - \omega_j)^2}{\sum_{v_i \in V(G)} \sum_{v_j \in V(G)} (\omega_i - \omega_j)^2} \mid \omega = (\omega_1, \omega_2, \dots, \omega_n) \in R^n, \omega \neq ae, \forall a \in R \right\}.$$

The second smallest Laplacian eigenvalue of a graph is called as the algebraic connectivity [16], which can be used to analyze the stability and synchronizability of the network. In the following, we will obtain some bounds of the second smallest p -Sombor Laplacian eigenvalue of graphs.

Theorem 3.3 *Let G be a connected graph with $|V(G)| = n$, $\mathcal{L}_p(G)$ and $\eta_1 > \eta_2 > \dots > \eta_s$ be defined as before.*

$$(1) \frac{n-1}{2} \eta_{s-1} \leq SO_p(G) = \frac{1}{2} \sum_{i=1}^s m(\eta_i) \eta_i \leq \frac{n-1}{2} \eta_1.$$

(2) *If $G = (X_1, X_2)$ is a bipartite graph and $|X_1| = n_1$, $|X_2| = n_2$, $n = n_1 + n_2$, then $\frac{n_1 n_2}{n} \eta_{s-1} \leq SO_p(G) \leq \frac{n_1 n_2}{n} \eta_1$.*

Proof. (1) By the definition of p -Sombor index $SO_p(G)$ and p -Sombor Laplacian matrix $\mathcal{L}_p(G)$, we have $SO_p(G) = \frac{1}{2} \sum_{v_i \in V(G)} \sum_{v_j \in V(G)} s_{ij}^p = \frac{1}{2} \text{tr}(\mathcal{L}_p(G)) = \frac{1}{2} \sum_{i=1}^s m(\eta_i) \eta_i$.

By Lemma 3.1, $\eta_s = 0$ and $m(\eta_s) = 1$. Thus $\frac{n-1}{2} \eta_{s-1} \leq \frac{1}{2} \sum_{i=1}^s m(\eta_i) \eta_i \leq \frac{n-1}{2} \eta_1$.

(2) Suppose that $\omega = (\omega_1, \omega_2, \dots, \omega_n) \in R^n$, where $\omega_i = 1$ if $v_i \in X_1$, $\omega_i = -1$ if $v_i \in X_2$. By Lemma 3.2, we have $\eta_1 \geq 2n \left\{ \frac{\sum_{v_i v_j \in E(G)} s_{ij}^p (\omega_i - \omega_j)^2}{\sum_{v_i \in V(G)} \sum_{v_j \in V(G)} (\omega_i - \omega_j)^2} \right\} = \frac{n}{4n_1 n_2} \sum_{v_i v_j \in E(G)} s_{ij}^p (\omega_i - \omega_j)^2 = \frac{n}{n_1 n_2} \sum_{v_i v_j \in E(G)} s_{ij}^p = \frac{n}{n_1 n_2} SO_p(G)$. So $SO_p(G) \leq \frac{n_1 n_2}{n} \eta_1$. Similarly, we have $SO_p(G) \geq \frac{n_1 n_2}{n} \eta_{s-1}$. ■

Lemma 3.4 *Let G be a graph with $|V(G)| = n$ and $|E(G)| = m$, the maximum degree Δ . Then*

$$(1) SO_p(G) \leq 2^{\frac{1}{p}} \Delta m;$$

$$(2) SO_p(G) \leq n^{\frac{1}{p}} \Delta^{1+\frac{1}{p}} m^{1-\frac{1}{p}}.$$

Proof. By Hölder inequality, we have

$$\left(\sum_{\substack{i \sim j \\ 1 \leq i, j \leq n}} ((d_i)^p + (d_j)^p)^{\frac{1}{p}} \cdot 1^{\frac{1}{q}} \right) \leq \left(\sum_{\substack{i \sim j \\ 1 \leq i, j \leq n}} ((d_i)^p + (d_j)^p) \right)^{\frac{1}{p}} \left(\sum_{\substack{i \sim j \\ 1 \leq i, j \leq n}} 1^q \right)^{\frac{1}{q}},$$

where $\frac{1}{p} + \frac{1}{q} = 1$. Then

$$\begin{aligned} \left(\sum_{\substack{i \sim j \\ 1 \leq i, j \leq n}} ((d_i)^p + (d_j)^p)^{\frac{1}{p}} \right)^p &\leq \left(\sum_{\substack{i \sim j \\ 1 \leq i, j \leq n}} ((d_i)^p + (d_j)^p) \right) m^{\frac{p}{q}} \\ &\leq 2m\Delta^p m^{\frac{p}{q}} \\ &= 2(\Delta m)^p. \end{aligned}$$

Thus $SO_p(G) \leq 2^{\frac{1}{p}} \Delta m$.

On the other hand, we have

$$\begin{aligned} \left(\sum_{\substack{i \sim j \\ 1 \leq i, j \leq n}} ((d_i)^p + (d_j)^p)^{\frac{1}{p}} \right)^p &\leq \left(\sum_{\substack{i \sim j \\ 1 \leq i, j \leq n}} ((d_i)^p + (d_j)^p) \right) m^{\frac{p}{q}} \\ &= \sum_{i=1}^n (d_i)^{p+1} m^{\frac{p}{q}} \\ &\leq n\Delta^{p+1} m^{\frac{p}{q}}. \end{aligned}$$

Thus $SO_p(G) \leq n^{\frac{1}{p}} \Delta^{1+\frac{1}{p}} m^{1-\frac{1}{p}}$. ■

By Theorem 3.3 and Lemma 3.4, we have

Corollary 3.5 *Let G be a graph with $|V(G)| = n$ and $|E(G)| = m$, the maximum (resp. minimum) degree Δ (resp. δ). Then*

- (1) $\sum_{i=1}^n \eta_i \leq \min\{2^{(1+\frac{1}{p})} \Delta m, 2n^{\frac{1}{p}} \Delta^{1+\frac{1}{p}} m^{1-\frac{1}{p}}\};$
- (2) $\eta_{n-1} \leq \min\{2^{(1+\frac{1}{p})} \frac{\Delta m}{n-1}, \frac{2}{n-1} n^{\frac{1}{p}} \Delta^{1+\frac{1}{p}} m^{1-\frac{1}{p}}\}.$

By Theorem 2.3 and Theorem 3.3, we have

Corollary 3.6 *Let G be a graph with $|V(G)| = n$ and $|E(G)| = m$, the maximum (resp. minimum) degree Δ (resp. δ). Then $\eta_1 \geq \frac{N_2}{2^{\frac{1}{p}} \Delta(n-1)}$ and $\eta_{n-1} \leq \frac{N_2}{2^{\frac{1}{p}} \delta(n-1)}$.*

4 Bounds of p -Sombor spectral radius and p -Sombor spectral spread

In the following, we obtain the relationship between the p -Sombor spectral radius ξ_1 and the adjacent spectral radius μ_1 .

Theorem 4.1 Let G be a graph with $|V(G)| = n$, the maximum (resp. minimum) degree Δ (resp. δ), ξ_1 be the p -Sombor spectral radius of G , μ_1 be the adjacent spectral radius of G . Then

$$2^{\frac{1}{p}}\delta\mu_1 \leq \xi_1 \leq 2^{\frac{1}{p}}\Delta\mu_1,$$

with equality if and only if G is a regular graph.

Proof. (1) Let $X = (x_1, x_2, \dots, x_n)$ be a unit eigenvector of $A = A(G)$ corresponding to μ_1 . Then

$$\begin{aligned} \xi_1 &\geq X^T \mathcal{S}_p X = 2 \sum_{\substack{i \sim j \\ 1 \leq i, j \leq n}} ((d_i)^p + (d_j)^p)^{\frac{1}{p}} x_i x_j \geq 2^{(1+\frac{1}{p})} \delta \sum_{\substack{i \sim j \\ 1 \leq i, j \leq n}} x_i x_j \\ &= 2^{\frac{1}{p}} \delta (X^T A X) = 2^{\frac{1}{p}} \delta \mu_1, \end{aligned}$$

with equality if and only if G is a regular graph.

(2) Let $Y = (y_1, y_2, \dots, y_n)$ be a unit eigenvector of $\mathcal{S}_p(G)$ corresponding to ξ_1 . Then

$$\begin{aligned} \xi_1 &= Y^T \mathcal{S}_p Y = 2 \sum_{\substack{i \sim j \\ 1 \leq i, j \leq n}} ((d_i)^p + (d_j)^p)^{\frac{1}{p}} y_i y_j \leq 2^{(1+\frac{1}{p})} \Delta \sum_{\substack{i \sim j \\ 1 \leq i, j \leq n}} y_i y_j \\ &= 2^{\frac{1}{p}} \Delta (Y^T A Y) \leq 2^{\frac{1}{p}} \Delta \mu_1, \end{aligned}$$

with equality if and only if G is a regular graph. ■

Theorem 4.2 Let G be a graph with $|V(G)| = n$, $|E(G)| = m$, the maximum (resp. minimum) degree Δ (resp. δ) and average degree \bar{d} , $M_1(G)$ be the first Zagreb index of G , $R(G)$ be the Randic index of G . Then

(1) $2^{1+\frac{1}{p}} \frac{m}{n} \delta \leq \xi_1 \leq 2^{\frac{1}{p}} (2m - n + 1)^{\frac{1}{2}} \Delta$, with left equality if and only if G is a regular graph, with right equality if and only if $G \cong K_n$.

(2) $2^{\frac{1}{p}} \left(\frac{M_1(G)}{n}\right)^{\frac{1}{2}} \delta \leq \xi_1 \leq 2^{\frac{1}{p}} \Delta^2$, with equality if and only if G is a regular graph.

(3) $\xi_1 \geq 2^{\frac{1}{p}} \delta \bar{d}$, with equality if and only if G is a \bar{d} regular graph.

(4) $\xi_1 \geq 2^{\frac{1}{p}} \frac{\delta}{m} R(G)$, with equality if and only if G is a regular graph.

Proof. (1) Since $\frac{2m}{n} \leq \mu_1 \leq \sqrt{2m - n + 1}$, with left equality iff G is a regular graph, with right equality if and only if $G \cong K_n$ [26]. Combining with Theorem 4.1, we have the conclusion.

(2) Since $\left(\frac{M_1(G)}{n}\right)^{\frac{1}{2}} \leq \mu_1 \leq \Delta$, with left equality if and only if G is a regular or semiregular graph, with right equality if and only if G is a regular graph [45]. Combining with Theorem 4.1, we have the conclusion.

(3) Since $\mu_1 \geq \bar{d} = \frac{2m}{n}$, with equality if and only if G is a \bar{d} -regular graph [20]. Combining with Theorem 4.1, we have the conclusion.

(4) Since $\mu_1 \geq \frac{R(G)}{m}$, with equality if and only if G is a regular graph [20]. Combining with Theorem 4.1, we have the conclusion. ■

Similar to the adjacent matrix or other non-negative matrices [14], for p -Sombor matrix, we also have the following similar result.

Lemma 4.3 *Let d be the diameter of G . If $S_p(G)$ has k distinct eigenvalues, then $k \geq d + 1$.*

Proof. Let $\xi_1, \xi_2, \dots, \xi_k$ be the k distinct eigenvalues of $S_p(G)$. Since $S_p(G)$ is a symmetric matrix, the minimal polynomial is

$$f(x) = (x - \xi_1)(x - \xi_2) \cdots (x - \xi_k) = x^k + a_1x^{k-1} + a_2x^{k-2} + \cdots + a_{k-1}x + a_k,$$

and there exists t such that

$$(S_p)^{k+t} + a_1(S_p)^{k+t-1} + a_2(S_p)^{k+t-2} + \cdots + a_{k-1}(S_p)^{t-1} + a_k(S_p)^t = 0,$$

where a_i ($1 \leq i \leq k$) are real numbers.

Let $a_{ij}^{(t)}$ (resp, $(s_{ij}^p)^{(t)}$) be the entries in the i -th row and j -th column of $A^t(G)$ (resp, $(S_p)^t(G)$). It is obvious that $(s_{ij}^p)^{(t)} = 0$ if and only if $a_{ij}^{(t)} = 0$.

Suppose that $k \leq d$, then there exist vertices v_i and v_j such that $a_{ij}^{(t)} = 0$ for any $t < d$ and $a_{ij}^{(d)} \neq 0$. Thus $(s_{ij}^p)^{(t)} = 0$ for any $t < d$ and $(s_{ij}^p)^{(d)} \neq 0$.

On the other hand, let $t = d - k$, since $(s_{ij}^p)^{(d-1)} = (s_{ij}^p)^{(d-2)} = \cdots = (s_{ij}^p)^{(d-k)} = 0$, and $(S_p)^{k+t} + a_1(S_p)^{k+t-1} + a_2(S_p)^{k+t-2} + \cdots + a_{k-1}(S_p)^{t-1} + a_k(S_p)^t = 0$, we have $(s_{ij}^p)^{(d)} = 0$, which is a contradiction. Thus $k \geq d + 1$. ■

Theorem 4.4 *Let G be a graph with $|V(G)| = n$. Then*

$$\xi_1 \leq \sqrt{\frac{(n-1)N_2}{n}}.$$

with equality if and only if $G \cong nK_1$ or $G \cong K_n$.

Proof. Since $\sum_{i=2}^n \xi_i^2 \leq (n-1) \sum_{i=2}^n \xi_i^2$, and $\sum_{i=1}^n \xi_i^2 = 2 \sum_{i \sim j} ((d_i)^p + (d_j)^p)^{\frac{2}{p}} = N_2$, then $\xi_1 \leq \sqrt{\frac{(n-1)N_2}{n}}$, with equality if and only if $\xi_2 = \xi_3 = \cdots = \xi_n$.

If $\xi_2 = \xi_3 = \cdots = \xi_n$, then by Lemma 4.3, we have the diameter $d \leq 1$, thus $G \cong nK_1$ or $G \cong K_n$. If $G \cong nK_1$, then $\xi_1 = 0 = \sqrt{\frac{(n-1)N_2}{n}}$; if $G \cong K_n$, then $\xi_1 = 2^{\frac{1}{p}}(n-1)^2 = \sqrt{\frac{(n-1)N_2}{n}}$. ■

Lemma 4.5 Let $a(\geq 0)$, $p(\geq 1)$ be constants and $f(x) = x^p + (a - x)^p$. Then $f(x)$ is monotonically decreasing when $x \leq \frac{a}{2}$, and $f(x)$ is monotonically increasing when $x \geq \frac{a}{2}$.

Proof. It is easy that $f'(x) = px^{p-1} - p(a - x)^{p-1} = p(x^{p-1} - (a - x)^{p-1})$.

If $x \leq \frac{a}{2}$, we have $f'(x) < 0$; if $x \geq \frac{a}{2}$, we have $f'(x) > 0$. Thus the conclusion holds. ■

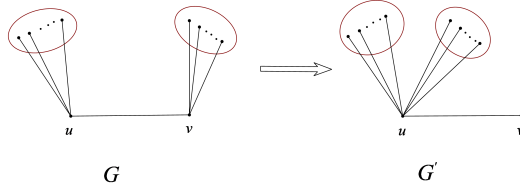


Figure 1. Transformation of Theorem 4.6.

Theorem 4.6 Let G be a connected graph, $e = uv$ be a cut (not pendent) edge of G . Suppose that X is the unit eigenvector of G corresponding to the p -Sombor spectral radius ξ_1 , i.e., $\mathcal{S}_p X = \xi_1 X$, and x_u is the component of X about the vertex u . Let $G' = G - \{vz | z \in N_G(v) \setminus \{u\}\} + \{uz | z \in N_G(v) \setminus \{u\}\}$ (see Figure 1), ξ'_1 be the p -Sombor spectral radius of G' . If $x_u \geq x_v$, then $\xi'_1 > \xi_1$.

Proof. By the Raleigh Quotient and Lemma 4.5, we have

$$\begin{aligned}
 \xi'_1 - \xi_1 &\geq X^T \mathcal{S}_p(G')X - X^T \mathcal{S}_p(G)X \\
 &= 2 \sum_{t \in N_G(u) \setminus \{v\}} [((d_t)^p + (d_u + d_v - 1)^p)^{\frac{1}{p}} - ((d_t)^p + (d_u)^p)^{\frac{1}{p}}] x_u x_t \\
 &\quad + 2 \sum_{z \in N_G(v) \setminus \{u\}} [((d_z)^p + (d_u + d_v - 1)^p)^{\frac{1}{p}} x_u - ((d_z)^p + (d_v)^p)^{\frac{1}{p}} x_v] x_z \\
 &\quad + 2[(1^p + (d_u + d_v - 1)^p)^{\frac{1}{p}} - ((d_u)^p + (d_v)^p)^{\frac{1}{p}}] x_u x_v \\
 &\geq 2 \sum_{t \in N_G(u) \setminus \{v\}} [((d_t)^p + (d_u + d_v - 1)^p)^{\frac{1}{p}} - ((d_t)^p + (d_u)^p)^{\frac{1}{p}}] x_u x_t \\
 &\quad + 2 \sum_{z \in N_G(v) \setminus \{u\}} [((d_z)^p + (d_u + d_v - 1)^p)^{\frac{1}{p}} - ((d_z)^p + (d_v)^p)^{\frac{1}{p}}] x_v x_z \\
 &\quad + 2[(1^p + (d_u + d_v - 1)^p)^{\frac{1}{p}} - ((d_u)^p + (d_v)^p)^{\frac{1}{p}}] x_u x_v > 0.
 \end{aligned}$$

By Theorem 4.6, we can obtain the sharp upper bounds of the p -Sombor spectral radius of trees immediately. ■

Theorem 4.7 *Let T be a tree with $|V(T)| = n$, $\xi_1(T)$ be the p -Sombor spectral radius of T . Then $\xi_1(T) \leq \xi_1(K_{1,n-1})$, with equality if and only if $T \cong K_{1,n-1}$.*

Results of Theorem 4.1, Theorem 4.6 and Theorem 4.7 extend the results of [30]. In the following, we consider the bounds of p -Sombor spectral spread of G .

Theorem 4.8 *Let G be a connected graph with $|V(T)| = n$, $\xi_1 \geq \xi_2 \geq \dots \geq \xi_n$ be the eigenvalues of $S_p(G)$. Then*

$$\xi_1 - \xi_n \leq 2 \sqrt{\sum_{v_i v_j \in E(G)} ((d_i)^p + (d_j)^p)^{\frac{2}{p}}} = \sqrt{2N_2}.$$

Proof. We know that $N_2 = \text{tr}((S_p)^2) = \xi_1^2 + \xi_2^2 + \dots + \xi_n^2 = 2 \sum_{v_i v_j \in E(G)} ((d_i)^p + (d_j)^p)^{\frac{2}{p}}$. Thus $\xi_n^2 \leq N_2 - \xi_1^2$, with equality iff $\xi_2 = \xi_3 = \dots = \xi_{n-1} = 0$ and $\xi_n = -\xi_1$. So $\xi_n \geq -\sqrt{N_2 - \xi_1^2}$. Thus $\xi_1 - \xi_n \leq \xi_1 + \sqrt{N_2 - \xi_1^2} \leq \sqrt{2N_2}$. ■

5 Bounds of p -Sombor energy and p -Sombor Estrada index

Let G be a simple graph, ξ_i ($i = 1, 2, \dots, n$) be the eigenvalues of p -Sombor matrix $S_p(G)$ and $\xi_1 \geq \xi_2 \geq \dots \geq \xi_n$, $S_p E = S_p E(G) = \sum_{i=1}^n |\xi_i|$ be the p -Sombor energy of G and $S_p EE = S_p EE(G) = \sum_{i=1}^n e^{\xi_i}$ be the p -Sombor Estrada index of G .

The following bounds of p -Sombor energy are similar to the (reduced) Sombor energy of Theorem 5.4 of [33], we omit the proof.

Theorem 5.1 *Let G be a simple graph with $|V(T)| = n$, the eigenvalues of $S_p(G)$ are $\xi_1 \geq \xi_2 \geq \dots \geq \xi_n$. Then*

- (1) $\sqrt{2N_2} \leq S_p E(G) \leq \sqrt{nN_2}$
- (2) $S_p E(G) \geq \sqrt{n(n-1)D^{\frac{2}{n}} + N_2}$, where $D = |\mu_1 \mu_2 \dots \mu_n| = |\det(S_p(G))|$.
- (3) $S_p E(G) \geq \frac{N_2 + n|\xi_1|\xi_n}{|\xi_1| + |\xi_n|}$.
- (4) $S_p E(G) \geq \frac{1}{2} \sqrt{4nN_2 - n^2(|\xi_1| - |\xi_n|)^2}$.
- (5) $S_p(G) \geq \sqrt{nN_2 - n \lfloor \frac{n}{2} \rfloor (1 - \frac{1}{n} \lfloor \frac{n}{2} \rfloor) (|\xi_1| - |\xi_n|)^2}$.

Theorem 5.2 *Let G be a simple graph with $|V(G)| = n$, $|E(G)| = m \geq 1$. Then*

$$S_p E(G) \geq \sqrt{\frac{(N_2)^3}{N_4}}.$$

Proof. By Hölder inequality, we have $\sum_{i=1}^n |\xi_i|^2 = \sum_{i=1}^n |\xi_i|^{\frac{2}{3}} (|\xi_i|^4)^{\frac{1}{3}} \leq (\sum_{i=1}^n |\xi_i|^{\frac{2}{3}}) (\sum_{i=1}^n |\xi_i|^4)^{\frac{1}{3}}$.

Since $S_p E(G) = \sum_{i=1}^n |\xi_i|$, $\sum_{i=1}^n \xi_i^2 = N_2$, and $\sum_{i=1}^n \xi_i^4 = N_4$. We get, $N_2 \leq (S_p E(G))^{\frac{2}{3}} (N_4)^{\frac{1}{3}}$, and then $S_p E(G) \geq \sqrt{\frac{(N_2)^3}{N_4}}$. ■

Theorem 5.3 *Let G be a simple graph with $|V(G)| = n$, $|E(G)| = m \geq 1$. Then*

$$S_p E(G) \geq \frac{(N_2)^2}{N_3}.$$

Proof. By Hölder inequality, we have $\sum_{i=1}^n |\xi_i|^2 = \sum_{i=1}^n |\xi_i|^{\frac{1}{2}} (|\xi_i|^3)^{\frac{1}{2}} \leq (\sum_{i=1}^n |\xi_i|^{\frac{1}{2}}) (\sum_{i=1}^n |\xi_i|^3)^{\frac{1}{2}}$.

Since $S_p E(G) = \sum_{i=1}^n |\xi_i|$, $\sum_{i=1}^n \xi_i^2 = N_2$, and $\sum_{i=1}^n \xi_i^3 = N_3$. We get, $N_2 \leq (S_p E(G))^{\frac{1}{2}} (N_3)^{\frac{1}{2}}$, and then $S_p E(G) \geq \frac{(N_2)^2}{N_3}$. ■

Compare the results of Theorems 5.2 and 5.3, we find that (1) if $\frac{N_3}{\sqrt{N_2 N_4}} > 1$, then the bound of Theorem 5.2 is better; (2) if $\frac{N_3}{\sqrt{N_2 N_4}} < 1$, then the bound of Theorem 5.3 is better; (3) if $\frac{N_3}{\sqrt{N_2 N_4}} = 1$, then the bound of Theorems 5.2 and 5.3 are the same.

Similar to the proof of Theorems 8, 15, 16, 24 and Corollary 12 of [9], we have the following results, we omit the proof.

Theorem 5.4 *Let G be a simple graph with $|V(G)| = n$. Then*

(1) $S_p EE(G) - S_p E(G) \leq n - 1 + e^{\sqrt{N_2}} - \sqrt{N_2} - \sqrt{2N_2}$, with equality if and only if $G \cong nK_1$.

(2) $S_p EE(G) + S_p E(G) \leq n - 1 + e^{S_p E(G)}$, with equality if and only if $G \cong nK_1$.

(3) $S_p E(G) \leq \sqrt{\frac{(3n-1)}{3} N_2}$, with equality if and only if $G \cong nK_1$.

(4) $S_p EE(G) \leq n - 1 + \frac{1}{2} N_2 + \frac{1}{6} N_3 - N_4^{\frac{1}{4}} - \frac{1}{2} N_4^{\frac{1}{2}} - \frac{1}{6} N_4^{\frac{3}{4}} + e^{N_4^{\frac{1}{4}}}$.

(5) $S_p EE(G) \geq \sqrt{n^2 + (\frac{1}{2} N_2)^2} + n N_2 + \frac{1}{3} n N_3 + \frac{1}{12} n N_4$.

Similar to the proof of Theorems 10, 11 of [39], we have the following results, we also omit the proof.

Theorem 5.5 *Let G be a simple graph with $|V(G)| = n$, n_+ , n_0 , n_- be the number of positive, zero, negative p -Sombor eigenvalues, respectively. Then*

(1) $\frac{1}{2}(e-1)S_p E(G) + n - n_+ \leq S_p EE(G) \leq n - 1 + e^{\frac{S_p E(G)}{2}}$, with both sides equality if and only if $G \cong nK_1$.

(2) $S_p EE(G) \geq e^{\xi_1} + n_0 + (n_+ - 1)e^{\frac{S_p E(G) - 2\xi_1}{2(n_+ - 1)}} + e^{-\frac{S_p E(G)}{2n_-}} n_-$.

In the following, we consider the bound of energy of subdivision graph of a k -regular graph, where the subdivision graph $S(G)$ is the graph obtained from G by adding one vertex for every edge of G .

Theorem 5.6 *Let G be a k -regular graph with $|V(G)| = n$, $|E(G)| = m$, $S(G)$ be the subdivision graph of G . Then*

$$S_p E(S(G)) \leq 2\sqrt{2}\sqrt{mn}(2^p + k^p)^{\frac{1}{p}}.$$

Proof. Let $Q(G)$ be the incident matrix of graph G . Then the p -Sombor matrix $S_p(S(G))$ can be written as

$$S_p(S(G)) = \begin{pmatrix} 0I_{n \times n} & (2^p + k^p)^{\frac{1}{p}} Q(G) \\ (2^p + k^p)^{\frac{1}{p}} Q^T(G) & 0I_{m \times m} \end{pmatrix}.$$

Suppose $\eta_1 \geq \eta_2 \geq \dots \geq \eta_{n+m}$ are the eigenvalues of the matrix $\begin{pmatrix} 0I_{n \times n} & Q(G) \\ Q^T(G) & 0I_{m \times m} \end{pmatrix}$, then we know that $\sum_{i=1}^{n+m} |\eta_i| \leq 2\sqrt{2}\sqrt{mn}$. Thus $S_p E(S(G)) \leq 2\sqrt{2}\sqrt{mn}(2^p + k^p)^{\frac{1}{p}}$. ■

6 Nordhaus-Gaddum-type results for p -Sombor spectral radius and energy

Lemma 6.1 [27] *Let $A = (a_{ij}), B = (b_{ij})$ be symmetric, non-negative matrices of order n . If $A \geq B$, i.e., $a_{ij} \geq b_{ij}$ for all i, j , then $\mu_1(A) \geq \mu_1(B)$.*

Lemma 6.2 [41] *Let G be a connected graph with $|V(G)| = n$. Then G has one positive eigenvalue in its adjacent spectrum if and only if G is a complete multipartite graph.*

Lemma 6.3 [4] *Let G be a graph with $|V(G)| = n$, $|E(G)| = m$, the maximum (resp. minimum) degree Δ (resp. $\delta \geq 1$). Then $\mu_1 \leq \sqrt{2m - \delta(n-1) + (\delta-1)\Delta}$.*

Lemma 6.4 *Let G be a graph with $|V(G)| = n$, $|E(G)| = m$ and the minimum degree δ . Then*

$$\xi_1 \geq \frac{2^{(1+\frac{1}{p})} \delta m}{n},$$

with equality if and only if G is a regular graph.

Proof. Suppose that $X = (x_1, x_2, \dots, x_n)^T$ be a unit vector. Then $\xi_1 \geq X^T S_p X = 2 \sum_{i \sim j} ((d_i)^p + (d_j)^p)^{\frac{1}{p}} x_i x_j \geq 2^{(1+\frac{1}{p})} \delta \sum_{i \sim j} x_i x_j$. Let $X = (\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}, \dots, \frac{1}{\sqrt{n}})^T$, then $\xi_1 \geq \frac{2^{(1+\frac{1}{p})} \delta m}{n}$. ■

Theorem 6.5 Let G be a graph with $|V(G)| = n$, $|E(G)| = m$, the maximum (resp. minimum) degree Δ (resp. $\delta \geq 1$). Then

$$\xi_1 \leq 2^{\frac{1}{p}} \Delta \sqrt{2m - \delta(n-1) + (\delta-1)\Delta},$$

with equality if and only if G is a regular graph.

Proof. By Lemmas 6.1 and 6.3, we have

$$\xi_1 \leq (\Delta^p + \Delta^p)^{\frac{1}{p}} \mu_1 \leq 2^{\frac{1}{p}} \Delta \sqrt{2m - \delta(n-1) + (\delta-1)\Delta},$$

with equality if and only if G is a regular graph. ■

Theorem 6.6 Let G be a graph with $|V(G)| = n$, $|E(G)| = m$. Then

$$S_p E(G) \geq \frac{2^{(2+\frac{1}{p})} \delta m}{n},$$

with equality if and only if $G \cong nK_1$ or G is a regular complete multipartite graph.

Proof. By Lemmas 6.2 and 6.4, we have

$$S_p E(G) = \sum_{i=1}^n |\xi_i| = 2 \sum_{i=1, \xi_i > 0}^n \xi_i \geq 2\xi_1 \geq \frac{2^{(2+\frac{1}{p})} \delta m}{n},$$

with equality if and only if $G \cong nK_1$ or G is a regular complete multipartite graph. ■

Theorem 6.7 Let G be a graph with $|V(G)| = n$, $|E(G)| = m$, the maximum (resp. minimum) degree Δ (resp. $\delta \geq 1$). Then

$$S_p E(G) \leq a + \sqrt{(n-1) \left(2^{(1+\frac{2}{p})} m \Delta^2 - a^2 \right)},$$

where $a = \max \left\{ \frac{2^{(1+\frac{1}{p})} \delta m}{n}, \Delta \sqrt{2^{(1+\frac{2}{p})} \frac{m}{n}} \right\}$.

Proof. By Lemma 6.4, we have $\xi_1 \geq \frac{2^{(1+\frac{1}{p})} \delta m}{n}$. By Cauchy-Schwartz inequality, we have

$$\sum_{i=2}^n |\xi_i| \leq \sqrt{(n-1) \left(\sum_{i=1}^n \xi_i^2 - \xi_1^2 \right)}.$$

On the other hand, $\sum_{i=1}^n \xi_i^2 = \text{tr}(\mathcal{S}_p^2) = 2 \sum_{i \sim j} ((d_i)^p + (d_j)^p)^{\frac{2}{p}} \leq 2^{(1+\frac{2}{p})} \Delta^2 m$, then

$$\sum_{i=2}^n |\xi_i| \leq \sqrt{(n-1) \left(2^{(1+\frac{2}{p})} m \Delta^2 - \xi_1^2 \right)}.$$

Thus $S_p E(G) = \sum_{i=1}^n |\xi_i| \leq \xi_1 + \sqrt{(n-1) \left(2^{(1+\frac{2}{p})} m \Delta^2 - \xi_1^2 \right)}$.

Let $f(a) = a + \sqrt{(n-1) \left(2^{(1+\frac{2}{p})} m \Delta^2 - a^2 \right)}$, by calculating, we have $\max\{f(a)\} = f\left(\Delta \sqrt{2^{(1+\frac{2}{p})} \frac{m}{n}}\right)$, for $a \in R$.

Thus $S_p E(G) \leq f(a)$, where $a = \max\left\{\frac{2^{(1+\frac{1}{p})\delta m}}{n}, \Delta \sqrt{2^{(1+\frac{2}{p})} \frac{m}{n}}\right\}$, a is the spectral radius of graph with $|V(G)| = n$, $|E(G)| = m$, the maximum (resp. minimum) degree Δ (resp. $\delta \geq 1$). ■

Theorem 6.8 *Let G be a graph with $|V(G)| = n$, $|E(G)| = m$, the maximum (resp. minimum) degree Δ (resp. δ). Then*

$$\xi_1 + \bar{\xi}_1 \geq \frac{2^{(1+\frac{1}{p})}}{n} (m\delta + (n-1-\Delta) \binom{n}{2} - m),$$

with equality if G is a regular graph.

Proof. Suppose that $X = (x_1, x_2, \dots, x_n)^T$ be a unit vector. Then

$$\begin{aligned} X^T (\mathcal{S}_p + \bar{\mathcal{S}}_p) X &= X^T \mathcal{S}_p X + X^T \bar{\mathcal{S}}_p X \\ &= 2 \sum_{v_i v_j \in E(G)} ((d_i)^p + (d_j)^p)^{\frac{1}{p}} x_i x_j + 2 \sum_{v_i v_j \in E(\bar{G})} ((\bar{d}_i)^p + (\bar{d}_j)^p)^{\frac{1}{p}} x_i x_j \\ &\geq 2^{(1+\frac{1}{p})} \delta \sum_{v_i v_j \in E(G)} x_i x_j + 2^{(1+\frac{1}{p})} (n-1-\Delta) \sum_{v_i v_j \in E(\bar{G})} x_i x_j. \end{aligned}$$

Let $X = (\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}, \dots, \frac{1}{\sqrt{n}})^T$. Then

$$\begin{aligned} X^T (\mathcal{S}_p + \bar{\mathcal{S}}_p) X &\geq 2^{(1+\frac{1}{p})} \frac{\delta}{n} \left(\sum_{v_i v_j \in E(G)} 1 \right) + 2^{(1+\frac{1}{p})} \frac{(n-1-\Delta)}{n} \left(\sum_{v_i v_j \in E(\bar{G})} 1 \right) \\ &= \frac{2^{(1+\frac{1}{p})}}{n} (m\delta + (n-1-\Delta) \binom{n}{2} - m). \end{aligned}$$

Thus, $\xi_1 + \bar{\xi}_1 \geq \frac{2^{(1+\frac{1}{p})}}{n} (m\delta + (n-1-\Delta) \binom{n}{2} - m)$. ■

Theorem 6.9 *Let G be a connected graph with $|V(G)| = n$, $|E(G)| = m$.*

(1) *If $\Delta(G) = n-1$ or $\delta(G) = n-1$, then*

$$\begin{aligned} \xi_1 + \bar{\xi}_1 &\leq 2^{\frac{1}{p}} \Delta(C_1) \sqrt{2|E(C_1)| - \delta(C_1)(|V(C_1)| - 1 - \Delta(C_1)) - \Delta(C_1)} \\ &\quad + 2^{\frac{1}{p}} (n-1) \sqrt{2m - n + 1}, \end{aligned}$$

where C_1 is the connected component of \overline{G} and $\xi_1(C_1) = \xi_1(\overline{G})$.

(2) If $\Delta(G) \leq n - 2$ and $\delta(G) \leq n - 2$, then

$$\begin{aligned} \xi_1 + \overline{\xi}_1 &\leq 2^{\frac{1}{p}}(n-1-\delta)\sqrt{2\binom{n}{2}-2m-(\delta+1)(n-1)+\delta(\Delta+1)} \\ &\quad + 2^{\frac{1}{p}}\Delta\sqrt{2m-\delta(n-1)+(\delta-1)\Delta}. \end{aligned}$$

Proof. (1) Let $\Delta(G) = n - 1$, $\delta(G) \geq 1$. Then \overline{G} is not a connected graph. By Lemma 6.5, we have $\xi_1 \leq 2^{\frac{1}{p}}(n-1)\sqrt{2m-\delta(n-1)+(\delta-1)(n-1)} = 2^{\frac{1}{p}}(n-1)\sqrt{2m-n+1}$.

Let C_1, C_2, \dots, C_t be the connected component of \overline{G} and $\xi_1(C_1) \geq \xi_1(C_2) \geq \dots \geq \xi_1(C_t)$. Then $\xi_1(\overline{G}) = \xi_1(C_1)$ and $\Delta(C_1) \leq \Delta(\overline{G}) \leq n - 2$. Thus

$$\overline{\xi}_1 = \xi_1(C_1) \leq 2^{\frac{1}{p}}\Delta(C_1)\sqrt{2|E(C_1)|-\delta(C_1)(|V(C_1)|-1-\Delta(C_1))-\Delta(C_1)}.$$

(2) In this case, G and \overline{G} are all connected graphs. By Lemma 6.5, we have

$$\xi_1 \leq 2^{\frac{1}{p}}\Delta\sqrt{2m-\delta(n-1)+(\delta-1)\Delta},$$

$$\begin{aligned} \overline{\xi}_1 &\leq 2^{\frac{1}{p}}\overline{\Delta}\sqrt{2\binom{n}{2}-2m-\delta(n-1)+(\delta-1)\overline{\Delta}} \\ &= 2^{\frac{1}{p}}(n-1-\delta)\sqrt{2\binom{n}{2}-2m-(\delta+1)(n-1)+\delta(\Delta+1)}. \end{aligned}$$

The proof is completed. ■

Theorem 6.10 *Let G be a connected graph with $|V(G)| = n$, $|E(G)| = m$, C_1, C_2, \dots, C_t be the connected component of \overline{G} and $\xi_1(C_1) \geq \xi_1(C_2) \geq \dots \geq \xi_1(C_t)$. Then*

$$S_p E(G) + S_p E(\overline{G}) \geq 2^{(2+\frac{1}{p})} \left(\frac{m\delta}{n} + \sum_{i=1}^t \frac{|E(C_i)|(|V(C_i)|-1-\Delta(C_i))}{|V(C_i)|} \right),$$

with equality if and only if G is a regular complete multipartite graph.

Proof. By Lemma 6.4, $\xi_1 \geq \frac{2^{(1+\frac{1}{p})}\delta m}{n}$, with equality iff G is a regular graph.

$$\begin{aligned} S_p E(G) + S_p E(\overline{G}) &= \sum_{i=1}^n |\xi_i| + \sum_{i=1}^n |\overline{\xi}_i| \\ &\geq 2\xi_1 + 2 \sum_{i=1}^t \xi_1(C_i) \\ &\geq 2^{(2+\frac{1}{p})} \frac{m\delta}{n} + 2^{(2+\frac{1}{p})} \sum_{i=1}^t \frac{|E(C_i)|(|V(C_i)|-1-\Delta(C_i))}{|V(C_i)|}. \end{aligned}$$

By Lemma 6.2 and Lemma 6.4, we have equality holds if and only if G is a regular complete multipartite graph. ■

7 Regression model for boiling point and some other invariants

In this section, we first investigate the relationship between boiling points (BP) of benzenoid hydrocarbons and Sombor spectral radius, Sombor energy. Then we consider the relationship between AcenFac (resp. Entropy, SNar, HNar) of octane isomers and Sombor spectral radius, Sombor energy. The 21 benzenoid hydrocarbons and 18 octane isomers are shown in Figure 2 and Figure 3. The experimental values of boiling points of benzenoid hydrocarbons of Table 1 are taken from [35]. The experimental values of AcenFac (resp. Entropy, SNar, HNar) of octane isomers of Table 2 are taken from [35] and [15]. With the data of Table 1, scatter plots between BP and Sombor spectral radius, Sombor energy are shown in Figure 4. We get the mathematical relationship-related coefficient (R) between boiling points and Sombor energy (resp. Sombor spectral radius) is about 0.9950 (resp. 0.8936), and

$$BP = 4.658 \times SE(G) + 31.24, \quad BP = 134.6 \times \xi_1(G) - 844,$$

where $SE(G)$, $\xi_1(G)$ are the Sombor energy, Sombor spectral radius of G , respectively.

On the other hand, with the data of Table 2, scatter plots between AcenFac (resp. Entropy, SNar, HNar) of octane isomers and Sombor spectral radius, Sombor energy are shown in Figure 5 and 6. And

$$AcenFac = -0.02465 \times \xi_1(G) + 0.5263, \quad Entropy = -2.978 \times \xi_1(G) + 128.4,$$

$$SNar = -0.2231 \times \xi_1(G) + 5.256, \quad HNar = -0.05843 \times \xi_1(G) + 1.86,$$

$$AcenFac = -0.021 \times SE(G) + 0.9109, \quad Entropy = -2.565 \times SE(G) + 175.7,$$

$$SNar = -0.19 \times SE(G) + 8.735, \quad HNar = -0.04981 \times SE(G) + 2.772.$$

From [43], we know that the correction coefficient (R) between boiling points of benzenoid hydrocarbons and eccentricity spectral radius is 0.7167, we compare the correction coefficient of Sombor spectral radius, Sombor energy with other spectral radius, energy, we find the Sombor energy (resp. Sombor spectral radius) is also a better predictor. The boiling points and Sombor energy is highly correlated since the correction coefficient (R) between boiling points of benzenoid hydrocarbons of Sombor energy is 0.9950. This points to the applicability of Sombor energy in QSPR analysis.

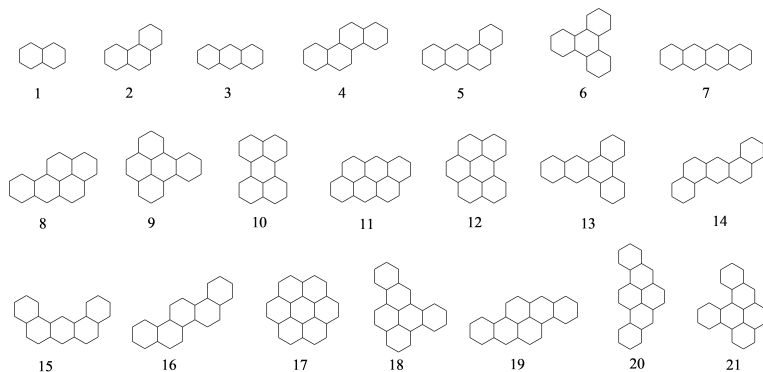


Figure 2. 21 benzenoid hydrocarbons.

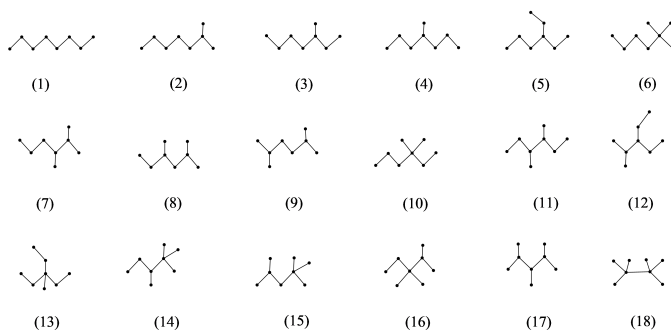


Figure 3. 18 octane isomers.

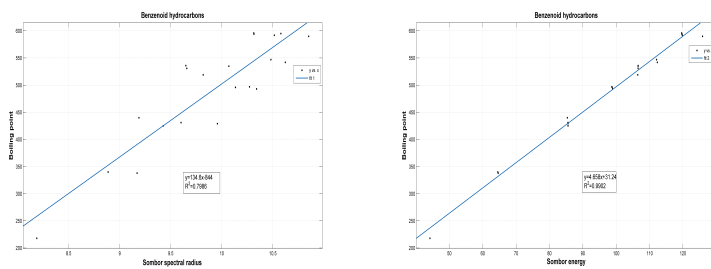


Figure 4. Scatter plot between BP of benzenoid hydrocarbons and $\xi_1(G)$ (resp. $SE(G)$).

Table 1. Experimental values of BP and Sombor spectral radius ($\xi_1(G)$), Sombor energy ($SE(G)$) of 21 benzenoid hydrocarbons

No.	BP($^{\circ}$ C)	$\xi_1(G)$	SE(G)	No.	BP($^{\circ}$ C)	$\xi_1(G)$	SE(G)
1	218	8.1882	44.1700	12	542	10.6216	112.3270
2	338	9.1702	64.6146	13	535	10.0690	106.5480
3	340	8.8866	64.5134	14	536	9.6476	106.5630
4	431	9.6008	85.5238	15	531	9.6571	106.5576
5	425	9.4256	85.5510	16	519	9.8174	106.4584
6	429	9.9568	85.5694	17	590	10.8507	125.8866
7	440	9.1885	85.3488	18	592	10.5141	119.8038
8	496	10.1336	98.8062	19	596	10.3127	119.6088
9	493	10.3400	98.9208	20	594	10.3144	119.7024
10	497	10.2712	98.6830	21	595	10.5782	119.6806
11	547	10.4807	112.0996				

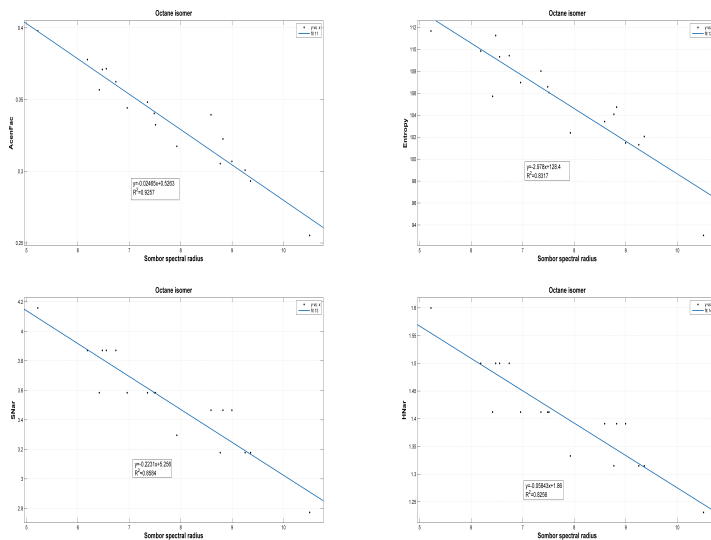


Figure 5. Scatter plot between AcenFac (resp. Entropy, SNar, HNar) of octane isomers and $\xi_1(G)$.

Table 2. Experimental values of AcenFac (resp. Entropy, SNar, HNar), $\xi_1(G)$ and $SE(G)$ of 18 octane isomers

No.	AcenFac	Entropy	SNar	HNar	$\xi_1(G)$	$SE(G)$
1	0.397898	111.67	4.159	1.6	5.2207	24.9204
2	0.377916	109.84	3.871	1.5	6.1862	25.4234
3	0.371002	111.26	3.871	1.5	6.4763	26.4694
4	0.371504	109.32	3.871	1.5	6.5533	25.2388
5	0.362472	109.43	3.871	1.5	6.7397	26.1798
6	0.339426	103.42	3.466	1.391	8.5905	27.8990
7	0.348247	108.02	3.584	1.412	7.3547	26.8572
8	0.344223	106.98	3.584	1.412	6.9600	26.7522
9	0.356830	105.72	3.584	1.412	6.4167	25.9628
10	0.322596	104.74	3.466	1.391	8.8227	27.8358
11	0.340345	106.59	3.584	1.412	7.4854	27.9238
12	0.332433	106.06	3.584	1.412	7.5110	26.5894
13	0.306899	101.48	3.466	1.391	8.9972	28.9882
14	0.300816	101.31	3.178	1.315	9.2535	29.3306
15	0.305370	104.09	3.178	1.315	8.7704	27.9486
16	0.293177	102.06	3.178	1.315	9.3598	29.4626
17	0.317422	102.39	3.296	1.333	7.9257	28.3642
18	0.255294	93.06	2.773	1.231	10.5096	30.7246

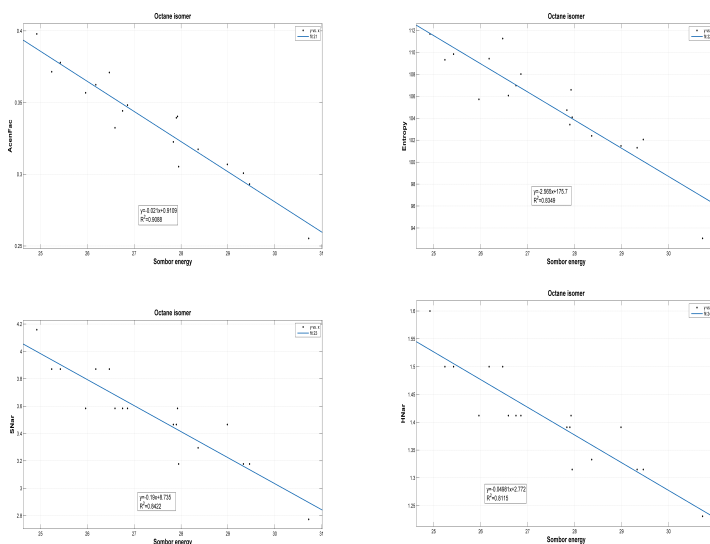


Figure 6. Scatter plot between AcenFac (resp. Entropy, SNar, HNar) of octane isomers and $SE(G)$.

8 Concluding Remarks

In this paper, we consider the properties of p -Sombor matrix. When $p = 2$ (resp. $p = 1$, $p = -1$), we can obtain most results of Sombor matrix (resp. first Zagreb matrix, ISI matrix). We determine the relationship between p -Sombor index $SO_p(G)$ and p -Sombor matrix $\mathcal{S}_p(G)$ by the k -th spectral moment N_k and spectral radius of $\mathcal{S}_p(G)$. Then we obtain some bounds of p -Sombor Laplacian eigenvalues, p -Sombor spectral radius, spectral spread, p -Sombor energy and p -Sombor Estrada index. We also study the Nordhaus-Gaddum-type results for p -Sombor spectral radius and energy. At last, we give the regression model for boiling point and some other invariants. We obtain the maximum trees for the p -Sombor spectral radius. The extremal unicyclic and bicyclic graphs for the p -Sombor spectral radius is also an interesting problem. Thus, we propose the following problems.

Problem 8.1 *Determine more properties of p -Sombor matrix.*

Problem 8.2 *What is the structure of the first three minimum (resp. maximum) trees, unicyclic and bicyclic graphs for the Sombor spectral radius?*

We intend to do exactly the above challenging problems in the near future.

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